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Quantum Computing for Quantum Simulation for NNSA Mission

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Beginning with Feynman in 1982, it was proposed that highly controllable quantum devices, later to become known as quantum computers, would be especially good at the simulation of other quantum systems. Around the turn of the 21st century, this notion was later formalized (by Lloyd and coworkers at MIT and Laflamme and coworkers at Los Alamos) to show how in particular instances, we expect an exponential speedup in the solution of the Schroedinger equation for chemical systems. Subsequently, quantum-accelerated quantum simulation for chemistry techniques have been developed by IBM, Google, Harvard, etc. This effort has led to the OpenFermion (openfermion.org, OF) community, an open source effort for compiling and analyzing quantum algorithms to simulate fermionic systems, including quantum chemistry. Among other functionalities, the current version of OF features data structures and tools for obtaining and manipulating representations of fermionic and qubit Hamiltonians. In October, 2017, the cover of Chemical and Engineering News posited “Quantum computers: Chemistry could be the machine’s killer app” for first principles understanding of biological systems and complex materials. Prof. Aspuru-Guzik (Harvard) predicts “I think that before 2035 QC will be beating classical computers at chemistry.” The algorithms at the heart of quantum chemistry codes (eigensolvers, fast fourier transforms) are the computation bottleneck.

As recently demonstrated in the **PEM** program, the results from quantum simulations have impacted both the **Equation of State** and **High Explosives** work. Quantum simulation also has the potential to speedup computationally intensive **Atomic Physics/Opacity** calculations that require the inclusion of an extreme number of states. The solid-state physics/band structure community has also shown interest in quantum simulation. The dynamic mean-field Theory (DMFT) [Kotliar-Vollhardt, 2004] when combined with the local density approximation (LDA) of density functional theory (DFT), has recently provided the first quantum many-body first-principles understanding of plutonium metal [Kotliar, 2006]. Plutonium, in its stable δ phase, is not well described within the LDA alone. That LDA approximation underestimates the phase volume by nearly 30% and predicts a nonexistent unstable phase. Using LDA+DMFT, researchers realized that the plutonium f electrons stabilize the material with the strong correlation effect [Savrasov-2001]. Furthermore, the approach has also predicted the vibration spectrum of δ -Pu [Dai, 2003], the essential feature of which compares well with the experimental results [Wong, 2003]. The researchers at the Los Alamos National

Laboratory were able to interpret the measured photoemission spectra on δ -Pu in terms of the quasiparticle peak and Hubbard bands described previously [Zhu, 2007]. More recently, the site-selection electronic correlation effects as revealed by the quasiparticle spectral density has been in α -Pu by the same LANL group [Zhu, 2013].

Quantum algorithms applied to the DMFT solver has been recently proposed by Microsoft and collaborators [Bauer, 2016]. While it has been shown that such a quantum computer can in principle solve certain small electronic structure problems and idealized model Hamiltonians, the highly relevant problem of directly solving a complex correlated material appears to require a prohibitive amount of resources. It was shown that by using a hybrid quantum-classical algorithm that incorporates the power of a small quantum computer into a framework of classical embedding algorithms, the electronic structure of complex correlated materials can be efficiently tackled using a quantum computer. The use of a quantum computer enables much larger and more accurate simulations than with any known classical algorithm, and will allow many open questions in quantum materials to be resolved once a small quantum computer with around 100 logical qubits becomes available.

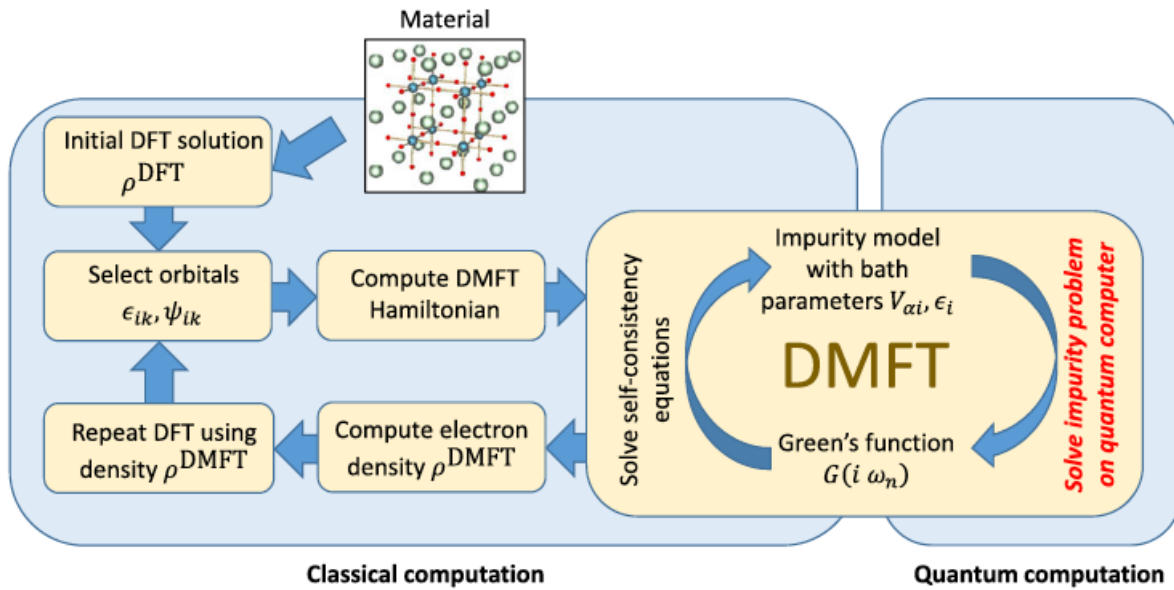


Figure 1. Quantum computation of the impurity solver for DMFT description of complex materials [Bauer, 2016]

Opacity. [Colgan, 2018] provides a short description of some recent work by that attempts to calculate opacities for elements with atomic numbers larger than zinc ($Z=30$). Such extensions are motivated by the continuing importance of accurate opacities and radiation transport models to other plasma studies found in inertial confinement fusion (ICF) research, industrial plasmas, and in the field of magnetic

confinement fusion. Some of these areas require models for elements that are not normally important in astrophysics research (such as Sn or W), and it is important to be able to provide accurate opacities for such systems.

At Los Alamos, atomic structure calculations are performed using the CATS code, a modern version of Cowan's codes. The calculations were carried out using the semi-relativistic Hartree-Fock, or HFR, option. For the Li-like, He-like and H-like ions of all elements discussed here, we use atomic data generated at a fine-structure level of detail including full configuration-interaction between all configurations. For all other ion stages, a mixed-UTA (MUTA) approach is used for all ions from Be-like through the neutral stage. The MUTA method retains all of the strongest fine-structure lines in a given transition array, which allows an accurate spectral description to be generated from a set of configuration-average populations. The generation of atomic data for a full level-resolved calculation is too computationally intensive at present.

Quantum chemistry. The atomic structure calculations necessary for opacities are closely related to the quantum chemistry calculations used for describing molecular structure. [Reiher, 2017] have shown that a quantum computer can be used to elucidate reaction mechanisms in complex chemical systems, using the open problem of biological nitrogen fixation in nitrogenase as an example. As is the case in pi-conjugated molecules or open-shell transition metal complexes, so-called strong static electron correlation plays a decisive role in the ground state. Such situations require multiconfigurational methods of which the complete-active-space self-consistent-field (CASSCF) approach has been established as a well-defined model that also serves as the basis for more advanced approaches. The work flow diagram for the CASSCF is very similar to that for the quantum DMFT simulations discussed above, where a proposed hybrid quantum-classical algorithm is proposed.

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